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FUNCTION SMOOTHING BY REPEATED AVERAGING

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General formulas for smooth univariate shape preserving approximation and allied accuracy preserving approximation are derived. Shape preserving properties of the smoothing operators are discussed, equivalent kernel forms are obtained, and thorough error analyses (with and without noise) are conducted for the smoothing operators and their derivatives. The class of functions to be approximated is the piecewise polynomials of possibly low smoothness.

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INTRODUCTION

Shapiro (ref 1) states in his introduction that he does not intend to discuss shape preserving properties of smoothing or iteration of the smoothing process. These are the topics which will be discussed here.

The basic objective in this report is to take a piecewise polynomial of low smoothness (having perhaps no derivatives) and replace it with an approximating function having any desired number of derivatives. One instance in which one might want to do this arises from computer-aided manufacturing where one might want to round off corners in piecewise linear geometries. Another instance arises from analysis of noisy data where one might want to reliably estimate the second derivative.

We will adhere to the idea of continuous smoothing through integration (as opposed to discrete smoothing through summation) because it becomes a trivial matter to interpolate in the smoothed function or any derivative thereof even for unequally spaced data.

SHAPE PRESERVATION PROPERTIES

Consider the averaging operator S defined by

$$S\{f(x)\} = \frac{1}{2h}\int_{x-h}^{x+h} f(t)dt = F_1(x)$$

First, the operator S is obviously linear because

$$S\{af(x) + bg(x)\} = \frac{1}{2h}\int_{x-h}^{x+h} af(t) + bg(t)dt$$

$$= a \cdot \frac{1}{2h}\int_{x-h}^{x+h} f(t)dt + b \cdot \frac{1}{2h}\int_{x-h}^{x+h} g(t)dt$$

$$= aS\{f(x)\} + bS\{g(x)\}$$

---

[1] Shapiro, H. S., Smoothing and Approximation of Functions, Van Nostrand Reinhold Company, New York, 1969.

Second, S preserves 1 and x because

$$S\{1\} = \frac{1}{2h}\int_{x-h}^{x+h} 1dt = \frac{t}{2h}\Big|_{x-h}^{x+h} = \frac{1}{2h}(x+h-(x-h)) = 1$$

and

$$S\{x\} = \frac{1}{2h}\int_{x-h}^{x+h} tdt = \frac{1}{2h}\frac{t^2}{2}\Big|_{x-h}^{x+h} = \frac{1}{4h}((x+h)^2-(x-h)^2)$$

$$= \frac{1}{4h}(x^2+2hx+h^2-(x^2-2hx+h^2)) = x$$

Therefore, S preserves all linear functions because

$$S\{A+Bx\} = S\{A\cdot 1+B\cdot x\} = AS\{1\} + BS\{x\} = A+Bx$$

This is the extent of S's accuracy preserving capabilities, however, because S does not preserve higher powers of x exactly:

$$S\{x^2\} = \frac{1}{2h}\int_{x-h}^{x+h} t^2dt = \frac{1}{2h}\frac{t^3}{3}\Big|_{x-h}^{x+h} = \frac{1}{6h}((x+h)^3-(x-h)^3)$$

$$= \frac{1}{6h}(x^3+3x^2h+3xh^2+h^3-(x^3-3x^2h+3xh^2-h^3)) = x^2 + \frac{h^2}{3}$$

Although the accuracy preserving ability of S is limited, it does have some nice shape preserving properties which no form of least squares approximation has. For instance, S preserves monotonicity. We can say, for example, that:

If f is monotone increasing on (A,B), then F_1 is monotone increasing on (A+h,B-h). Proof: Assume f is monotone increasing on (A,B), i.e.,

$$A < x < y < B \;\Rightarrow\; f(x) \leq f(y)$$
(implies)

Let

$$A + h < a \leq b < B - h$$

By definition,

$$F_1(a) = \frac{1}{2h}\int_{a-h}^{a+h} f(t)dt = \frac{1}{2h}\int_{b-h}^{b+h} f(t-(b-a))dt$$

In the second integral,

$$b-h \leqslant t \leqslant b+h$$

Therefore

$$A < a-h \leqslant b-h \leqslant t \leqslant b+h < B$$

and

$$A < a-h \leqslant t - (b-a) \leqslant a+h \leqslant b+h < B$$

We therefore have

$$A < t - (b-a) < t < B$$

Since f is monotone increasing on (A,B), we also have

$$f(t-(b-a)) \leqslant f(t)$$

The second integral is therefore bounded above by

$$\frac{1}{2h} \int_{b-h}^{b+h} f(t)dt$$

but this is just $F_1(b)$. We finally conclude that

$$F_1(a) \leqslant F_1(b)$$

and that F_1 is monotone increasing on (A+h,B-h).

S also preserves convexity or concavity "away from" inflection points in the following sense:

If f"(x) exists and is positive for A < x < B, then $F_1''(x) > 0$ for A+h < x < B-h. Proof: Assume f"(x) exists and f"(x) > 0 for A < x < B. Take arbitrary x in (A+h,B-h). Therefore

$$x-h > A \quad \text{and} \quad x+h < B$$

Now for $x - h \leqslant t \leqslant x + h$, we have A < t < B and f"(t) > 0. Therefore

$$\int_{x-h}^{x+h} f''(t)dt = f'(x+h) - f'(x-h) > 0$$

But by definition,

$$S\{f(x)\} = F_1(x) = \frac{1}{2h} \int_{x-h}^{x+h} f(t)dt$$

Using Leibnitz's rule for differentiating integrals, we have

$$F_1'(x) = \frac{1}{2h} (f(x+h)-f(x-h))$$

and differentiating again, we have

$$F_1''(x) = \frac{1}{2h} (f'(x+h)-f'(x-h))$$

and

$$F_1''(x) > 0$$

on (A+h,B-h).

S also preserves positivity in the following sense:

If $f(x) > 0$ on (A,B), then $S\{f(x)\} > 0$ on (A+h,B-h). Proof: Assume $f(x) > 0$ on (A,B). Take x arbitrary in (A+h,B-h). Therefore $x-h > A$ and $x+h < B$. Now if $A < x-h \leqslant t \leqslant x+h < B$, we have $f(t) > 0$ and also that

$$\int_{x-h}^{x+h} f(t)dt > 0$$

Therefore

$$S\{f(x)\} > 0$$

on (A+h,B-h). A corollary to this theorem is that

$$f(x) > g(x) \text{ on } (A,B) \Rightarrow S\{f(x)\} > S\{g(x)\}$$

on (A+h,B-h). (S is a monotone operator.)

Proof: Assume $f(x) > g(x)$ on (A,B). Therefore

$$f(x) - g(x) > 0 \quad \text{on } (A,B)$$

and

$$S\{f(x) - g(x)\} > 0 \quad \text{on } (A+h,B-h)$$

Linearity of S gives us $S\{f(x)\} > S\{g(x)\}$.

We can summarize the preceding theorems by the form:

If $f(x)$ has property P on (A,B), then $S\{f(x)\}$ has property P on (A+h,B-h). If we think of repeating the application of S to f i times (S^i), we can easily prove that

$$
\begin{array}{c}
f(x) \text{ has P on } (A,B) \\
\Rightarrow \\
S^i\{f(x)\} \text{ has P on } (A+ih,B-ih)
\end{array}
$$

These shape preserving properties are important for applications in industrial computer-aided design and manufacturing, and in data analysis situations when one or more derivatives must be estimated.

REPEATED AVERAGING

We may apply the smoothing operator S repeatedly in order to obtain approximations of higher smoothness in the following manner:

$$S\{f(x)\} = \frac{1}{2h} \int_{x-h}^{x+h} f(t)dt = F_1(x)$$

$$F_{i+1}(x) = S\{F_i(x)\} \quad i \geq 1$$

In order to carry out this process, we must be able to compute the successive indefinite integrals of f

$$f_o(x) = f(x)$$

$$f_{i+1}(x) = \int_a^x f_i(t)dt \quad i \geq 0$$

We now compute the first few F's

$$F_1(x) = \frac{1}{2h} \int_{x-h}^{x+h} f(t)dt = \frac{1}{2h} (f_1(x+h)-f_1(x-h))$$

$$F_2(x) = \frac{1}{2h}\int_{x-h}^{x+h} F_1(t)dt = \frac{1}{2h}\int_{x-h}^{x+h} \frac{1}{2h}(f_1(t+h)-f_1(t-h))dt$$

$$= \frac{1}{(2h)^2}\left\{\int_{x-h}^{x+h} f_1(t+h)dt - \int_{x-h}^{x+h} f_1(t-h)dt\right\}$$

$$= \frac{1}{(2h)^2}\left\{f_2(x+2h) - f_2(x) - (f_2(x)-f_2(x-2h))\right\}$$

$$= \frac{1}{(2h)^2}\left\{f_2(x+2h) - 2f_2(x) + f_2(x-2h)\right\}$$

$$F_3(x) = \frac{1}{2h}\int_{x-h}^{x+h} F_2(t)dt = \frac{1}{2h}\int_{x-h}^{x+h} \frac{1}{(2h)^2}\left\{f_2(t+2h) - 2f_2(t) + f_2(t-2h)\right\}dt$$

$$= \frac{1}{(2h)^3}\left\{\int_{x-h}^{x+h} f_2(t+2h)dt - 2\int_{x-h}^{x+h} f_2(t)dt + \int_{x-h}^{x+h} f_2(t-2h)dt\right\}$$

$$= \frac{1}{(2h)^3}\left\{f_3(x+3h) - f_3(x+h) - 2(f_3(x+h)-f_3(x-h)) + f_3(x-h) - f_3(x-3h)\right\}$$

$$= \frac{1}{(2h)^3}\left\{f_3(x+3h) - 3f_3(x+h) + 3f_3(x-h) - f_3(x-3h)\right\}$$

The appearance of the binomial coefficients is fairly evident, and we can guess the general formula for the ith smooth as

$$F_i(x) = \frac{1}{(2h)^i}\sum_{k=0}^{i} (-1)^k\binom{i}{k}f_i(x+(i-2k)h,$$

All we need to do to prove this formula in general (by mathematical induction) is to be sure that it is true for $i = 1$, and be able to conclude that it is true for $i+1$ on the assumption that it is true for i. For $i = 1$, we have

$$F_1(x) = \frac{1}{(2h)^1}\sum_{k=0}^{1} (-1)^k\binom{1}{k}f_1(x+(1-2k)h) = \frac{1}{2h}(f_1(x+h)-f_1(x-h))$$

which we have already shown to be true.

By definition,

$$F_{i+1}(x) = \frac{1}{2h}\int_{x-h}^{x+h} F_i(t)dt$$

Assuming the result for i,

$$F_{i+1}(x) = \frac{1}{2h} \int_{x-h}^{x+h} \frac{1}{(2h)^i} \sum_{k=0}^{i} (-1)^k \binom{i}{k} f_i(t+(i-2k)h)dt$$

$$= \frac{1}{(2h)^{i+1}} \sum_{k=0}^{i} (-1)^k \binom{i}{k} \int_{x-h}^{x+h} f_i(t+(i-2k)h)dt$$

$$= \frac{1}{(2h)^{i+1}} \sum_{k=0}^{i} (-1)^k \binom{i}{k} \{f_{i+1}(x+h+(i-2k)h) - f_{i+1}(x-h+(i-2k)h)\}$$

$$F_{i+1}(x) = \frac{1}{(2h)^{i+1}} \sum_{k=0}^{i} (-1)^k \binom{i}{k} \{f_{i+1}(x+(i+1-2k)h) - f_{i+1}(x+(i-1-2k)h)\}$$

$$= \frac{1}{(2h)^{i+1}} \{ \sum_{k=0}^{i} (-1)^k \binom{i}{k} f_{i+1}(x+(i+1-2k)h) - \sum_{k=0}^{i} (-1)^k \binom{i}{k} f_{i+1}(x+(i-1-2k)h)\}$$

$$= \frac{1}{(2h)^{i+1}} \{ \sum_{k=0}^{i} (-1)^k \binom{i}{k} f_{i+1}(x+(i+1-2k)h)$$

$$- \sum_{k=1}^{i+1} (-1)^{k-1} \binom{i}{k-1} f_{i+1}(x+(i-1-2(k-1))h)\}$$

$$= \frac{1}{(2h)^{i+1}} \{ \sum_{k=0}^{i} (-1)^k \binom{i}{k} f_{i+1}(x+(i+1-2k)h) + \sum_{k=1}^{i+1} (-1)^k \binom{i}{k-1} f_{i+1}(x+(i+1-2k)h)\}$$

At this point we must mention the well-known recursion for the binomial coefficients

$$\binom{i}{k-1} + \binom{i}{k} = \binom{i+1}{k}$$

from which we immediately conclude that

$$\binom{i}{-1} = 0 = \binom{i}{i+1}$$

by substituting k = 0 and i+1 in the recursion.

These last two facts enable us to extend the ranges of summation of our two sums appropriately

$$F_{i+1}(x) = \frac{1}{(2h)^{i+1}} \left\{ \sum_{k=0}^{i+1} (-1)^k \binom{i}{k} f_{i+1}(x+(i+1-2k)h) \right.$$

$$\left. + \sum_{k=0}^{i+1} (-1)^k \binom{i}{k-1} f_{i+1}(x+(i+1-2k)h) \right\}$$

Therefore

$$F_{i+1}(x) = \frac{1}{(2h)^{i+1}} \sum_{k=0}^{i+1} (-1)^k \left\{ \binom{i}{k} + \binom{i}{k-1} \right\} f_{i+1}(x+(i+1-2k)h)$$

$$= \frac{1}{(2h)^{i+1}} \sum_{k=0}^{i+1} (-1)^k \binom{i+1}{k} f_{i+1}(x+(i+1-2k)h)$$

We have concluded that our general result holds for i+1 if it holds for i, and the proof is complete.

Having established the validity of the formula for the ith smooth of f,

$$F_i(x) = \frac{1}{(2h)^i} \sum_{k=0}^{i} (-1)^k \binom{i}{k} f_i(x+(i-2k)h)$$

we may trivially obtain the jth derivative of F_i merely by subtracting j from the subscript of f.

$$F_i^{(j)}(x) = \frac{1}{(2h)^i} \sum_{k=0}^{i} (-1)^k \binom{i}{k} f_{i-j}(x+(i-2k)h)$$

If f is not differentiable (and usually it won't be), we must be sure that $i \geqslant j$.

Suppose we wanted to estimate the second derivative of f. We would of course need $j = 2$. Suppose in addition, we wanted the second derivative to be smooth to the extent of being differentiable. The lowest value of i that we could use would depend on the smoothness of f. If f were continuous, then f_1 would be differentiable and we would need $i = 3$ (at least). If f were discontinuous, however, f_2 would be differentiable and we would need $i = 4$.

SMOOTHING ERROR AND CONVERGENCE

In this section, our goal is to obtain a general result describing the convergence of the jth derivative of the ith iterated smooth of a sufficiently smooth function. The following formula for integration-by-parts will be used a number of times:

$$\int_a^b f(x)g(x)dx = f(b)\int_a^b g(x)dx - \int_a^b f'(x)\int_a^x g(t)dtdx$$

In addition, *Leibnitz's rule for differentiating an integral containing a parameter* will subsequently be used.

$$\frac{d}{dx}\int_{\alpha(x)}^{\beta(x)} f(t,x)dt = \int_{\alpha(x)}^{\beta(x)} \frac{\partial}{\partial x} f(t,x)dt + f(\beta(x),x)\beta'(x) - f(\alpha(x),x)\alpha'(x)$$

By definition,

$$S\{f(x)\} = \frac{1}{2h}\int_{x-h}^{x+h} f(t)dt$$

Letting D be the derivative operator, we have by Leibnitz's rule for differentiating integrals:

$$DSf(x) = \frac{1}{2h}\left(f(x+h) - f(x-h)\right)$$

but

$$Df(x) = f'(x)$$

and

$$SDf(x) = \frac{1}{2h} \int_{x-h}^{x+h} f'(t)dt$$

$$= \frac{1}{2h} (f(x+h) - f(x-h))$$

$$= DS\ f(x)$$

We therefore have commutativity of the S and D operators for differentiable f:

$$SD = DS$$

It is easy to show that in general, $S^iD^j = D^jS^i$ for sufficiently smooth f.

The commutativity of the smoothing and derivative operators tells us that when we apply the smoothing operator to a function, we simultaneously apply the same operator to all available derivatives of the function. This in turn tells us that the shape preserving properties of the smoothing operator extend to all derivatives as well.

Recalling

$$F_{i+1}^{(j)}(x) = \frac{1}{2h} \int_{x-h}^{x+h} F_i^{(j)}(t)dt \qquad j \geqslant 0$$

we rewrite

$$2hF_{i+1}^{(j)}(x) = \int_{x-h}^{x} F_i^{(j)}(t)dt - \int_{x+h}^{x} F_i^{(j)}(t)dt$$

Using integration-by-parts on these two integrals, we have

$$2hF_{i+1}^{(j)}(x) = F_i^{(j)}(x)\int_{x-h}^{x} dt - \int_{x-h}^{x} F_i^{(j+1)}(t)\int_{x-h}^{t} dudt$$

$$- \{F_i^{(j)}(x)\int_{x+h}^{x} dt - \int_{x+h}^{x} F_i^{(j+1)}(t)\int_{x+h}^{t} dudt\}$$

$$= hF_i^{(j)}(x) - \int_{x-h}^{x} F_i^{(j+1)}(t)(t-x+h)dt$$

$$+ hF_i^{(j)}(x) + \int_{x+h}^{x} F_i^{(j+1)}(t)(t-x-h)dt$$

Therefore, we get

$$2h(F_{i+1}^{(j)}(x)-F_i^{(j)}(x)) = -\int_{x-h}^{x} F_i^{(j+1)}(t)(t-x+h)dt + \int_{x+h}^{x} F_i^{(j+1)}(t)(t-x-h)dt$$

Using integration-by-parts again on each integral, we have

$$2h(F_{i+1}^{(j)}(x)-F_i^{(j)}(x)) = -\Big\{F_i^{(j+1)}(x)\int_{x-h}^{x} t-x+h\ dt$$

$$-\int_{x-h}^{x} F_i^{(j+2)}(t)\int_{x-h}^{t} u-x+h\ dudt\Big\} + F_i^{(j+1)}(x)\int_{x+h}^{x} t-x-h\ dt$$

$$-\int_{x+h}^{x} F_i^{(j+2)}(t)\int_{x+h}^{t} u-x-h\ dudt$$

$$2h(F_{i+1}^{(j)}(x)-F_i^{(j)}(x)) = -F_i^{(j+1)}(x)\ \frac{(t-x+h)^2}{2}\Bigg|_{t=x-h}^{x}$$

$$+\int_{x-h}^{x} F_i^{(j+2)}(t)\ \frac{(u-x+h)^2}{2}\Bigg|_{u=x-h}^{t} dt + F_i^{(j+1)}(x)\ \frac{(t-x-h)^2}{2}\Bigg|_{t=x+h}^{x}$$

$$-\int_{x+h}^{x} F_i^{(j+2)}(t)\ \frac{(u-x-h)^2}{2}\Bigg|_{u=x+h}^{t} dt$$

$$= -\frac{h^2}{2} F_i^{(j+1)}(x) + \int_{x-h}^{x} F_i^{(j+2)}(t)\ \frac{(t-x+h)^2}{2}\ dt$$

$$+\frac{h^2}{2} F_i^{(j+1)}(x) - \int_{x+h}^{x} F_i^{(j+2)}(t)\ \frac{(t-x-h)^2}{2}\ dt$$

$$= \int_{x-h}^{x} F_i^{(j+2)}(t)\ \frac{(t-x+h)^2}{2}\ dt + \int_{x}^{x+h} F_i^{(j+2)}(t)\ \frac{(t-x-h)^2}{2}\ dt$$

Using the absolute value triangle inequalities (for sums and integrals), we have

$$2h\left|F_{i+1}^{(j)}(x) - F_i^{(j)}(x)\right| \le \int_{x-h}^{x} \left|F_i^{(j+2)}(t)\right| \frac{(t-x+h)^2}{2}\ dt$$

$$+\int_{x}^{x+h} \left|F_i^{(j+2)}(t)\right| \frac{(t-x-h)^2}{2}\ dt$$

We must now define the following function norm:

$$\|g\|_{(x;h)} = \text{least upper bound of the set } \{|g(t)| : x-h \leq t \leq x+h\}$$

$$= \max \{|g(t)| : x-h \leq t \leq x+h\}$$

if g is continuous.

Employing this norm, the previous inequality gives us

$$2h\left|F_{i+1}^{(j)}(x) - F_i^{(j)}(x)\right| \leq \tfrac{1}{2}\|F_i^{(j+2)}\|_{(x;h)}\left(\int_{x-h}^{x} (t-x+h)^2 dt + \int_{x}^{x+h} (t-x-h)^2 dt\right)$$

$$= \tfrac{1}{2}\|F_i^{(j)}\|_{(x;h)}\left(\frac{h^3}{3} - \frac{(-h)^3}{3}\right) = \frac{h^3}{3}\|F_i^{(j+2)}\|_{(x;h)}$$

Therefore, we have another preliminary result

$$\left|F_{i+1}^{(j)}(x) - F_i^{(j)}(x)\right| \leq \frac{h^2}{6}\|F_i^{(j+2)}\|_{(x;h)}$$

The special case of i = j = 0 gives us

$$\left|S\{f(x)\} - f(x)\right| \leq \frac{h^2}{6}\|f''\|_{(x;h)}$$

which substantiates our previously obtained result that the smoothing approximation is exact for all linear functions. Before we proceed to our general results, however, we need just two more preliminary results. The first norm theorem is:

If $\|f\|_{(x;h)} \leq \|g\|_{(x;k)}$, then $\|f\|_{(x;h+\ell)} \leq \|g\|_{(x;k+\ell)}$ where x is arbitrary and h, k, $\ell \geq 0$. Proof: Assume $\|f\|_{(x;h)} \leq \|g\|_{(x;k)}$. By definition,

$$\begin{aligned}\|f\|_{(x;h+\ell)} &= \max\{|f(t)| : x-(h+\ell) \leq t \leq x+h+\ell\}\\ &= \max\{\|f\|_{(t;h)} : x-\ell \leq t \leq x+\ell\}\\ &\leq \max\{\|g\|_{(t;k)} : x-\ell \leq t \leq x+\ell\}\\ &= \max\{|g(t)| : x-(k+\ell) \leq t \leq x+k+\ell\}\\ &= \|g\|_{(x;k+\ell)}\end{aligned}$$

We now follow the first norm theorem with the second norm theorem:

$$\|F_{i+1}^{(j)}\|_{(x;kh)} \leq \|F_i^{(j)}\|_{(x;(k+1)h)}$$

Proof: Since

$$F_{i+1}^{(j)}(x) = \frac{1}{2h} \int_{x-h}^{x+h} F_i^{(j)}(t)dt$$

Taking absolute values and using the norm, we have

$$|F_{i+1}^{(j)}(x)| \leq \frac{1}{2h} \int_{x-h}^{x+h} |F_i^{(j)}(t)|\, dt$$

$$\leq \frac{1}{2h} \|F_i^{(j)}\|_{(x;h)} \int_{x-h}^{x+h} dt = \|F_i^{(j)}\|_{(x;h)}$$

but

$$|F_{i+1}^{(j)}(x)| = \|F_{i+1}^{(j)}\|_{(x;0)}$$

Therefore

$$\|F_{i+1}^{(j)}\|_{(x;0)} \leq \|F_i^{(j)}\|_{(x;h)}$$

and using the first norm theorem, we have

$$\|F_{i+1}^{(j)}\|_{(x;kh)} \leq \|F_i^{(j)}\|_{(x;(k+1)h)}$$

We are now prepared to establish the main result of the section. Subtracting and adding the intermediate smooths, we have

$$F_i^{(j)}(x) - f^{(j)}(x) = F_i^{(j)}(x) - F_{i-1}^{(j)}(x) + F_{i-1}^{(j)}(x)$$
$$- F_{i-2}^{(j)}(x) + F_{i-2}^{(j)}(x) - \ldots - F_1^{(j)}(x) + F_1^{(j)}(x) - f^{(j)}(x)$$

Taking absolute values and using the absolute value triangle inequality for sums, we have

$$|F_i^{(j)}(x) - f^{(j)}(x)| \leq |F_i^{(j)}(x) - F_{i-1}^{(j)}(x)|$$

$$+ |F_{i-1}^{(j)}(x) - F_{i-2}^{(j)}(x)| + \ldots + |F_1^{(j)}(x) - f^{(j)}(x)|$$

(note that use of the triangle inequality does not make this inequality particularly strong, since the arguments of the absolute values will tend to have the same sign), but we have already proved that

$$\left| F_{i+1}^{(j)}(x) - F_i^{(j)}(x) \right| \leq \frac{h^2}{6} \| F_i^{(j+2)} \|_{(x;h)}$$

Using this fact in the previous sum, we get

$$\left| F_i^{(j)}(x) - f^{(j)}(x) \right| \leq \frac{h^2}{6} \left(\| F_{i-1}^{(j+2)} \|_{(x;h)} + \| F_{i-2}^{(j+2)} \|_{(x;h)} + \ldots + \| f^{(j+2)} \|_{(x;h)} \right)$$

Now, applying the second norm theorem to the first term i-1 times, to the second term i-2 times etc., we have

$$\left| F_i^{(j)}(x) - f^{(j)}(x) \right| \leq \frac{h^2}{6} \left(\| f^{(j+2)} \|_{(x;ih)} + \| f^{(j+2)} \|_{(x;(i-1)h)} + \ldots + \| f^{(j+2)} \|_{(x;h)} \right)$$

Since the first term is obviously the largest, we have our final result for sufficiently smooth f

$$\left| F_i^{(j)}(x) - f^{(j)}(x) \right| \leq \frac{ih^2}{6} \| f^{(j+2)} \|_{(x;ih)}$$

This result tells us that the derivatives of the ith smooth converge just as fast (quadratically in h) as the ith smooth itself. Also, since

$$\| f^{(j+2)} \|_{(x;ih)} \leq \| f^{(j+2)} \|_{(x;\infty)}$$

and

$$\| f^{(j+2)} \|_{(x;\infty)}$$

is really independent of x, the convergence of the ith smooth and all its derivatives is uniform. Subsequently, we will discover that this error bound for the jth derivative of the ith smooth is the best possible (smallest).

HIGHER ACCURACY SMOOTHING

We now show how to obtain formulas of higher accuracy using the repeated smoothing operator S^i. Unfortunately, in the process of obtaining higher accuracy, we must give up the shape preserving properties of our approximations.

Assume in what follows that f(x) is a polynomial of degree n. We know by definition that

$$S\{f(x)\} = F_1(x) = \frac{1}{2h}\int_{x-h}^{x+h} f(t)dt$$

Expanding f(t) in a Taylor series around x gives us

$$F_1(x) = \frac{1}{2h}\int_{x-h}^{x+h} \sum_{k=0}^{n} \frac{f^{(k)}(x)}{k!} (t-x)^k dt$$

$$= \frac{1}{2h} \sum_{k=0}^{n} \frac{f^{(k)}(x)}{k!} \cdot \left.\frac{(t-x)^{k+1}}{k+1}\right|_{t=x-h}^{x+h}$$

$$= \frac{1}{2h} \sum_{k=0}^{n} \frac{f^{(k)}(x)}{(k+1)!} (h^{k+1}-(-h)^{k+1})$$

$$= \frac{1}{2h} \sum_{k=0}^{n} \frac{f^{(k)}(x)h^{k+1}}{(k+1)!} (1-(-1)^{k+1})$$

It is clear that every other element of this sum is zero (k odd). If we let G(x) be the greatest integer $\leqslant$ x, we have

$$F_1(x) = \sum_{k=0,2,4,\ldots,2G(n/2)} \frac{f^{(k)}(x)h^k}{(k+1)!}$$

$$= \sum_{k=0}^{G(n/2)} \frac{f^{(2k)}(x)h^{2k}}{(2k+1)!}$$

Letting

$$m = G(\frac{n}{2})$$

and

$$C_k^1 = \frac{h^{2k}}{(2k+1)!}$$

where the superscripts on the C's denote the smooth index, we have

$$F_1(x) = \sum_{k=0}^{m} C_k^1 f^{(2k)}(x)$$

Since F_1 is also a polynomial of degree n, as well as all successive F's, we can write

$$F_i(x) = \sum_{k=0}^{m} C_k^i f^{(2k)}_{(x)}$$

and

$$F_{i+1}(x) = \sum_{k=0}^{m} C_k^{i+1} f^{(2k)}_{(x)} = \sum_{j=0}^{m} C_j^1 F_i{}^{(2j)}_{(x)}$$

but

$$F_i^{(2j)}(x) = \sum_{k=0}^{m-j} C_k^i f^{(2k+2j)}_{(x)} = \sum_{k=j}^{m} C_{k-j}^i f^{(2k)}_{(x)}$$

Therefore

$$F_{i+1}(x) = \sum_{k=0}^{m} C_k^{i+1} f^{(2k)}_{(x)} = \sum_{j=0}^{m} C_j^1 \sum_{k=j}^{m} C_{k-j}^i f^{(2k)}_{(x)}$$

$$= \sum_{j=0}^{m} \sum_{k=j}^{m} C_j^1 C_{k-j}^i f^{(2k)}_{(x)}$$

Carefully interchanging the order of summation in this double sum, we have

$$F_{i+1}(x) = \sum_{k=0}^{m} C_k^{i+1} f^{(2k)}_{(x)} = \sum_{k=0}^{m} \sum_{j=0}^{k} C_j^1 C_{k-j}^i f^{(2k)}_{(x)}$$

$$= \sum_{k=0}^{m} f^{(2k)}_{(x)} \sum_{j=0}^{k} C_j^1 C_{k-j}^i$$

We therefore conclude that

$$C_k^{i+1} = \sum_{j=0}^{k} C_j^1 C_{k-j}^i$$

We have

$$C_o^{i+1} = C_o^1 C_o^i$$

$$C_1^{i+1} = C_o^1 C_1^i + C_1^1 C_o^i$$

$$C_2^{i+1} = C_o^1 C_2^i + C_1^1 C_1^i + C_2^1 C_o^i$$

$$\vdots$$

$$C_m^{i+1} = C_o^1 C_m^i + C_1^1 C_{m-1}^i + \ldots + C_m^1 C_o^i$$

So if we define the semi-convolution product of vectors a and b as

$$a \cdot b = (a_o, a_1, a_2, \ldots a_m) \cdot (b_o, b_1, b_2, \ldots b_m)$$

$$= (a_o b_o, a_o b_1 + a_1 b_o, a_o b_2 + a_1 b_1 + a_2 b_o, \ldots$$

$$a_o b_m + a_1 b_{m-1} + \ldots + a_m b_o)$$

we can write $C^{i+1} = C^1 \cdot C^i$, where removal of the subscript denotes a vector.

We use the term "semi-convolution" because the dimensionality of the product is the same as that of the factors. Also note that $C_o^i = 1$ for all i.

Let us now derive an approximating operator which is exact for cubics. Let $f(x)$ be a cubic polynomial ($n=3$). Thus, we have $m = 1$. We can write the following two equations and subsequently eliminate $f''(x)$:

$$F_i(x) = f(x) + C_1^i f''(x)$$

$$F_{i+1}(x) = f(x) + C_1^{i+1} f''(x)$$

But first,

$$C^{i+1} = (1, C_1^{i+1}) = C^1 \cdot C^i$$

$$= (1, C_1^1) \cdot (1, C_1^i)$$

$$= (1, C_1^i + C_1^1)$$

Therefore

$$C_1^{i+1} = C_1^i + C_1^1$$

or

$$C_1^{i+1} - C_1^i = C_1^1$$

Summing both sides of this equation, we have

$$\sum_{i=1}^{k} (C_1^{i+1} - C_1^i) = \sum_{i=1}^{k} C_1^1$$

$$C_1^{k+1} - C_1^1 = kC_1^1$$

$$C_1^{k+1} = (k+1)C_1^1$$

Therefore

$$C_1^i = iC_1^1$$

We have

$$F_i(x) = f(x) + iC_1^1 f''(x)$$

and

$$F_{i+1}(x) = f(x) + (i+1)C_1^1 f''(x)$$

Eliminating $f''(x)$

$$F_{i+1}(x) - \frac{i+1}{i} F_i(x) = f(x) - \frac{i+1}{i} f(x)$$

$$iF_{i+1}(x) - (i+1)F_i(x) = if(x) - (i+1)f(x)$$

Therefore

$$\begin{aligned} f(x) &= (i+1)F_i(x) - iF_{i+1}(x) \\ &= (i+1)S^i f(x) - iS^{i+1} f(x) \end{aligned}$$

and we have a smoothing operator which is exact for all cubic polynomials

$$s_3 = (i+1)S^i - iS^{i+1}$$

We will now obtain an operator which is exact for all quintic polynomials.

Since $n = 5$, $m = 2$, and we write

$$F_i(x) = f(x) + C_1^i f''(x) + C_2^i f^{(4)}(x)$$

$$F_{i+1}(x) = f(x) + C_1^{i+1} f''(x) + C_2^{i+1} f^{(4)}(x)$$

$$F_{i+2}(x) = f(x) + C_1^{i+2} f''(x) + C_2^{i+2} f^{(4)}(x)$$

We simply eliminate $f''(x)$ and $f^{(4)}(x)$ from these equations, leaving $f(x)$ defined in terms of the three smooths. First, however, we get the formulas for the C's.

$$\begin{aligned} C^{i+1} &= (1, C_1^{i+1}, C_2^{\,i+1}) = C^1 \cdot C^i \\ &= (1, C_1^1, C_2^1) \cdot (1, C_1^i, C_2^i) \\ &= (1, C_1^i + C_1^1, C_2^i + C_1^1 C_1^i + C_2^1) \end{aligned}$$

Therefore

$$C_1^{i+1} = C_1^i + C_1^1$$

and

$$C_2^{i+1} = C_2^i + C_1^1 C_1^i + C_2^1$$

As before,

$$C_1^i = iC_1^1$$

but

$$C_2^{i+1} - C_2^i = i(C_1^1)^2 + C_2^1$$

Summing both sides, we have

$$\sum_{i=1}^{k} C_2^{i+1} - C_2^i = (C_1^1)^2 \sum_{i=1}^{k} i + \sum_{i=1}^{k} C_2^1$$

$$C_2^{k+1} - C_2^1 = \frac{k(k+1)}{2} (C_1^1)^2 + kC_2^1$$

$$C_2^{k+1} = \frac{k(k+1)}{2} (C_1^1)^2 + (k+1)C_2^1$$

Therefore

$$C_2^i = \frac{i(i-1)}{2} (C_1^1)^2 + iC_2^1$$

Using these C's to eliminate $f''(x)$ and $f^{(4)}(x)$ ultimately gives us

$$f(x) = ½((i+1)(i+2)F_i(x) - 2i(i+2)F_{i+1}(x) + i(i+1)F_{i+2}(x))$$

Our smoothing operator which preserves quintics is therefore

$$s_5 = ½((i+1)(i+2)S^i - 2i(i+2)S^{i+1} + i(i+1)S^{i+2})$$

Using s_3 and s_5 as examples, we can guess that the operator

$$s_{2k+1} = i\binom{i+k}{k} \sum_{j=0}^{k} (-1)^j \binom{k}{j} \frac{S^{i+j}}{i+j}$$

is exact for all polynomials of degree 2k+1 and has $O(h^{2k+2})$ error. It is interesting to note that these s operators are generalizations of Tukey's (ref 2) method of twicing. Tukey uses the notation, data = smooth + rough, which we

[2]Tukey, J. W., Exploratory Data Analysis, Addison-Wesley, New York, 1977.

will abbreviate as $d = m + r$. He then defines the first smooth as $m_1 = Sd$, and subsequent iterated smooths by $m_{i+1} = m_i + Sr_i$, where $r_i = d - m_i$. Eliminating r_i, we get $m_{i+1} = Sd + m_i - Sm_i$. For twicing, we have

$$\begin{aligned} m_2 &= Sd + m_1 - Sm_1 \\ &= Sd + Sd - S^2 d \\ &= (2S-S^2)d \end{aligned}$$

For thricing, we have

$$\begin{aligned} m_3 &= Sd + m_2 - Sm_2 \\ &= Sd + (2S-S^2)d - S(2S-S^2)d \\ &= (S+2S-S^2-2S^2+S^3)d \\ &= (3S-3S^2+S^3)d \end{aligned}$$

The twicing and thricing operators are the same as s_3 and s_5 with $i = 1$. Note, however, that we have made use of the linearity of our smoothing operator S, while Tukey (ref 2) does not restrict himself to linear operators.

KERNEL FORM

We can easily write the first smooth in kernel form

$$S\{f(x)\} = \int_{x-h}^{x+h} \frac{1}{2h} f(t)dt = \int_{-\infty}^{\infty} K_1(t-x)f(t)dt$$

where

$$K_1(t) = \begin{cases} \frac{1}{2h} & -h \leq t \leq h \\ 0 & \text{elsewhere} \end{cases}$$

We will generalize this form to i successive smooths and find $K_i(t)$ where

$$S^i\{f(x)\} = \int_{-\infty}^{\infty} K_i(t-x)f(t)dt$$

We will need the following simple theorem regarding successive integrations of f:

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[2]Tukey, J. W., Exploratory Data Analysis, Addision-Wesley, New York, 1977.

$$f_i(x) = \int_a^x f(t)\,\frac{(x-t)^{i-1}}{(i-1)!}\,dt$$

We prove this theorem by mathematical induction.

By definition,

$$f_1(x) = \int_a^x f(t)dt$$

hence, our formula is true for $i = 1$. Also by definition,

$$f_{i+1}(x) = \int_a^x f_i(u)du$$

On the assumption that our formula is true for i, we have

$$f_{i+1}(x) = \int_a^x \int_a^u f(t)\,\frac{(u-t)^{i-1}}{(i-1)!}\,dtdu$$

Interchanging the order of integration gives us

$$f_{i+1}(x) = \int_a^x \int_t^x f(t)\,\frac{(u-t)^{i-1}}{(i-1)!}\,dudt$$

$$= \int_a^x f(t)\,\frac{(u-t)^{i}}{i!}\,\Big|_{u=t}^{u=x}\,dt$$

$$= \int_a^x f(t)\,\frac{(x-t)^{i}}{i!}\,dt$$

Hence, our formula is true for $i+1$ also, and the theorem is proved.

Now, we have already proved that

$$S^i f(x) = \sum_{k=0}^{i} \frac{(-1)^k}{(2h)^i}\binom{i}{k} f_i(x+(i-2k)h)$$

Therefore

$$S^i f(x) = \sum_{k=0}^{i} \frac{(-1)^k}{(2h)^i} \binom{i}{k} \int_a^{x+(i-2k)h} f(t) \frac{(x+(i-2k)h-t)^{i-1}}{(i-1)!} dt$$

$$= \sum_{k=0}^{i} \int_a^{x+(i-2k)h} \frac{(-1)^k}{(2h)^i (i-1)!} \binom{i}{k} (x+(i-2k)h-t)^{i-1} f(t) dt$$

$$= \sum_{k=0}^{i} \int_a^{x+(i-2k)h} g_k(t) dt$$

where

$$g_k(t) = \frac{(-1)^k}{(2h)^i (i-1)!} \binom{i}{k} (x+(i-2k)h-t)^{i-1} f(t)$$

We may specify a arbitrarily, as long as it is independent of k. Let $a = x - ih$, hence

$$S^i f(x) = \sum_{k=0}^{i} \int_{x-ih}^{x+(i-2k)h} g_k(t) dt$$

$$= \sum_{k=0}^{i-1} \int_{x-ih}^{x+(i-2k)h} g_k(t) dt$$

$$S^i f(x) = \sum_{k=0}^{i-1} \int_{-ih}^{(i-2k)h} g_k(t+x) dt$$

$$= \sum_{k=0}^{i-1} \int_{-ih}^{(i-2k)h} G_k(t) dt$$

where $G_k(t) = g_k(t+x)$.

Writing out some of the terms of this sum, we have

$$S^i f(x) = \int_{-ih}^{ih} G_o(t)dt + \int_{-ih}^{(i-2)h} G_1(t)dt + \int_{-ih}^{(i-4)h} G_2(t)dt$$

$$+ \int_{-ih}^{(i-6)h} G_3(t)dt + \ldots + \int_{-ih}^{-(i-2)h} G_{i-1}(t)dt$$

Rewriting this sum as a sum of integrals over disjoint ranges, we have

$$S^i f(x) = \int_{(i-2)h}^{ih} G_o(t)dt + \int_{(i-4)h}^{(i-2)h} G_o(t) + G_1(t)dt$$

$$+ \int_{(i-6)h}^{(i-4)h} G_o(t) + G_1(t) + G_2(t)dt$$

$$+ \ldots + \int_{-ih}^{-(i-2)h} G_o(t) + G_1(t) + \ldots + G_{i-1}(t)dt$$

Hence

$$S^i f(x) = \sum_{k=0}^{i-1} \int_{(i-2(k+1))h}^{(i-2k)h} \sum_{j=0}^{k} G_j(t)dt$$

$$= \sum_{k=0}^{i-1} \int_{(i-2(k+1))h}^{(i-2k)h} \sum_{j=0}^{k} g_j(t+x)dt$$

$$= \sum_{k=0}^{i-1} \int_{(i-2(k+1))h}^{(i-2k)h} \sum_{j=0}^{k} \frac{(-1)^j}{(2h)^i(i-1)!} \binom{i}{j} ((i-2j)h-t)^{i-1} f(t+x)dt$$

$$= \sum_{k=0}^{i-1} \int_{(i-2(k+1))h}^{(1-2k)h} f(t+x) \frac{1}{(2h)^i(i-1)!} \sum_{j=0}^{k} (-1)^j \binom{i}{j} ((i-2j)h-t)^{i-1} dt$$

but we want

$$S^i f(x) = \int_{x-ih}^{x+ih} K_i(t-x)f(t)dt$$

$$= \int_{-ih}^{ih} K_i(t)f(t+x)dt$$

We can therefore conclude that for $0 \leq k \leq i-1$ and $(i-2(k+1))h \leq t \leq (i-2k)h$,

$$K_i(t) = \frac{1}{(2h)^i (i-1)!} \sum_{j=0}^{k} (-1)^j \binom{i}{j} ((i-2j)h-t)^{i-1}$$

We see that K_i is a piecewise polynomial of degree $i-1$. In fact, K_i is a B-spline (ref 3) area normalized to unity with constant mesh spacing 2h.

Note that for $k = 0$ $((i-2)h \leq t \leq ih)$,

$$K_i(t) \propto (ih-t)^{i-1}$$

Hence

$$K_i^{(j)}(t) \propto (ih-t)^{i-j-1}$$

and

$$K_i^{(j)}(ih) = 0 \text{ for } j \leq i-2$$

ERROR ANALYSIS WITH NOISE

Let D^j denote the taking of the jth derivative with respect to x, and ℓf denote the piecewise linear approximation to f over a uniform mesh with mesh width τ. The error in our estimate of the jth derivative of f is given by

$$e_j(x) = f^{(j)}(x) - D^j S^i \ell(f+\epsilon)(x)$$

where, in order to compute our estimate of $f^{(j)}$, we take the sum of the underlying function f and noise ϵ, evaluate this over a discrete mesh (take data), define a piecewise linear approximation to the data, smooth the approximation, and take the jth derivative of the smooth.

We may rewrite $e_j(x)$ in the following manner:

$$\begin{aligned} e_j(x) &= f^{(j)}(x) - D^j S^i (\ell f(x) + \ell\epsilon(x)) \\ &= f^{(j)}(x) - D^j S^i \ell f(x) - D^j S^i \ell\epsilon(x) \end{aligned}$$

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[3]de Boor, C., A Practical Guide to Splines, Springer-Verlag, New York, 1978.

but

$$D^jS^i\ell f(x) = D^jS^i(\ell f(x)-f(x)+f(x)) = D^jS^if(x) - D^jS^i(f(x)-\ell f(x))$$

Therefore

$$e_j(x) = f^{(j)}(x) - D^jS^if(x) + D^jS^i(f(x)-\ell f(x)) - D^jS^i\ell\epsilon(x)$$

The first two terms denote the component of error due to smoothing alone. The next term denotes the component of error due to linear interpolation of f, and the last term denotes the component of error due to noise, i.e., the stochastic component. We denote the first three terms by A(x), the analytic or deterministic component, and the last term by R(x), the random or stochastic component.

Thus, we can abbreviate

$$e_j(x) = A(x) - R(x)$$

We also let E_a, E_q, and V denote the arithmetic mean, quadratic mean, and variance operators, respectively.

By definition, the local quadratic mean error is given by

$$E_q(e_j(x)) = (E_a(e_j(x)^2))^{\frac{1}{2}} = q_j(x)$$

Therefore

$$q_j(x)^2 = E_a(A(x)^2-2A(x)R(x)+R(x)^2) = A(x)^2 - 2A(x)E_a(R(x)) + E_a(R(x)^2)$$

but

$$\begin{aligned} R(x) &= D^jS^i\ell\epsilon(x) \\ &= D^j\int_{x-ih}^{x+ih} K_i(t-x)\ell\epsilon(t)dt \\ &= \int_{x-ih}^{x+ih} (-1)^jK_i^{(j)}(t-x)\ell\epsilon(t)dt \end{aligned}$$

(using Leibnitz's rule and the fact that $K_i^{(j)}(\pm ih) = 0$ for $j \leq i-2$).

Approximating the integral by a sum over the sampled data we get:

$$R(x) \sim (-1)^j \sum_k K_i^{(j)}(t_k-x)\epsilon(t_k)\tau$$

The expected value of this sum is clearly zero, and using elementary statistical theory for the variance of a linear combination of independent random variables gives us

$$V(R(x)) \sim \sum_k K_i^{(j)}(t_k-x)^2\sigma^2\tau^2 = \sigma^2\tau \sum_k K_i^{(j)}(t_k-x)^2\tau$$

Re-approximating the sum by an integral, we have

$$V(R(x)) \sim \sigma^2\tau \int_{x-ih}^{x+ih} K_i^{(j)}(t-x)^2dt = \sigma^2\tau \int_{-ih}^{ih} K_i^{(j)}(t)^2dt$$

This approximation will be good for τ small relative to h.

Since $E_a(R(x)) = 0$, $E_a(R(x)^2) = V(R(X))$, and we have

$$q_j(x)^2 = A(x)^2 + V(R(x))$$

where

$$V(R(x)) \sim \sigma^2\tau\int_{-ih}^{ih} K_i^{(j)}(t)^2dt$$

and σ^2 is the variance of the noise.

Now

$$A(x) = f^{(j)}(x) - D^jS^if(x) + D^jS^i(f(x)-\ell f(x))$$

and taking absolute values gives

$$|A(x)| \leq |f^{(j)}(x) - D^jS^if(x)| + |D^jS^i(f(x)-\ell f(x))|$$

The previously obtained bound on the first term is given by

$$|f^{(j)}(x) - D^jS^if(x)| \leq \frac{ih^2}{6} \|f^{(j+2)}\|_{(x;ih)}$$

We now obtain a bound on the linear interpolation part

$$|D^j S^i(f(x)-\ell f(x))| = |D^j \int_{x-ih}^{x+ih} K_i(t-x)(f(t)-\ell f(t))dt|$$

$$= |\int_{x-ih}^{x+ih} K_i^{(j)}(t-x)(f(t)-\ell f(t))dt| \leq \int_{x-ih}^{x+ih} |K_i^{(j)}(t-x)|\,|f(t) - \ell f(t)|\,dt$$

but from elementary interpolation theory, we know that

$$|f(t) - \ell f(t)| \leq \frac{\tau^2}{8} \|f''\|_{(t;\tau)}$$

So

$$|D^j S^i(f(x)-\ell f(x))| \leq \frac{\tau^2}{8} \int_{x-ih}^{x+ih} |K_i^{(j)}(t-x)|\,\|f''\|_{(t;\tau)}dt$$

$$\leq \frac{\tau^2}{8} \|f''\|_{(x;ih+\tau)} \int_{x-ih}^{x+ih} |K_i^{(j)}(t-x)|\,dt = \frac{\tau^2}{8} \|f''\|_{(x;ih+\tau)} \int_{-ih}^{ih} |K_i^{(j)}(t)|\,dt$$

and we have approximate bounds on the local quadratic mean error in our estimate of the jth derivative of f:

$$q_j(x)^2 \leq \{\frac{ih^2}{6} \|f^{(j+2)}\|_{(x;ih)} + \frac{\tau^2}{8} \|f''\|_{(x;ih+\tau)} \int_{-ih}^{ih} |K_i^{(j)}(t)|\,dt\}^2$$

$$+ \sigma^2\tau \int_{-ih}^{ih} K_i^{(j)}(t)^2 dt$$

Let

$$I = \int_{-ih}^{ih} |K_i^{(j)}(t)|\,dt$$

and

$$J = \int_{-ih}^{ih} K_i^{(j)}(t)^2 dt$$

and approximate

$$\|f^{(j+2)}\|_{(x;ih)} \sim |f^{(j+2)}(x)| + ih\,|f^{(j+3)}(x)|$$

$$\|f''\|_{(x;ih+\tau)} \sim |f''(x)| + (ih+\tau)|f'''(x)|$$

We therefore have the approximate local bound

$$q_j(x)^2 \lesssim \left\{\frac{ih^2}{6}\left(\left|\overset{(j+2)}{f(x)}\right| + ih\left|\overset{(j+3)}{f(x)}\right|\right)\right.$$

$$\left. + \frac{\tau^2 I}{8}\left(\left|f''(x)\right| + (ih+\tau)\left|f'''(x)\right|\right)\right\}^2 + \sigma^2\tau J$$

and the approximate global bound

$$q_j^2 = \frac{1}{L}\int_0^L q_j(x)^2 dx \lesssim \frac{1}{L}\int_0^L \left\{\frac{ih^2}{6}\left(\left|\overset{(j+2)}{f(x)}\right| + ih\left|\overset{(j+3)}{f(x)}\right|\right)\right.$$

$$\left. + \frac{\tau^2 I}{8}\left(\left|f''(x)\right| + (ih+\tau)\left|f'''(x)\right|\right)\right\}^2 dx + \sigma^2\tau J$$

At this point, we will consider the problem of estimating I and J (at least for $j = 0,1,2$). Obviously, we do not want to go to the trouble of evaluating the integrals of squares or absolute values of derivatives of higher order B splines, so we will do an asymptotic development. First, we note that the B spline kernel functions (K_j) appear in an entirely different context - namely in the statistical theory of obtaining probability distributions of sums of independent, uniformly distributed random variables (ref 4). If $x_1, x_2, \ldots x_i$ have K_1 as their common probability density and we define y_i by

$$y_i = \sum_{k=1}^{i} x_k$$

then y_i will have K_i as its probability density.

We can easily compute the variance of y_i

$$V(y_i) = \sigma_i^2 = \sum_{k=1}^{i} V(x_k) = iV(x)$$

[4]Cramer, H., Mathematical Methods of Statistics, Princeton University Press, New Jersey, 1946.

but x has density K_1, therefore $E_a(x) = 0$, and

$$V(x) = E_a(x^2) = \int_{-h}^{h} \frac{x^2}{2h}\,dx = \left.\frac{x^3}{6h}\right|_{-h}^{h} = \frac{h^2}{3}$$

We then have

$$\sigma_i{}^2 = \frac{ih^2}{3}$$

We now bring to bear the central limit theorem of statistics, which tells us that the probability distribution of y_i will approach the normal distribution as i becomes large. In practice, this normality approximation is rather good, even for small i. We can therefore write

$$K_i(t) \sim \frac{1}{\sqrt{2\pi}\,\sigma_i}\, e^{-\frac{1}{2}(t/\sigma_i)^2}$$

for large i. First, we need a couple of derivatives of K_i:

$$K_i'(t) = -\frac{t}{\sigma_i{}^2} K_i(t)$$

and

$$K_i''(t) = \frac{1}{\sigma_i{}^2}\left(\left(\frac{t}{\sigma_i}\right)^2 - 1\right)K_i(t)$$

The incomplete gamma function is defined by

$$\gamma(a,x) = \int_0^x t^{a-1}e^{-t}dt$$

We will subsequently need a recursion formula for γ. Using integration-by-parts, we get

$$\gamma(a,x) = x^{a-1}\int_0^x e^{-t}dt - \int_0^x (a-1)t^{a-2}\int_0^t e^{-u}du\,dt$$

$$= x^{a-1} \cdot -e^{-t}\Big|_0^x - \int_0^x (a-1)t^{a-2} \cdot -e^{-u}\Big|_0^t dt$$

$$= x^{a-1}(1-e^{-x}) - \int_0^x (a-1)t^{a-2}(1-e^{-t})dt$$

$$= x^{a-1}(1-e^{-x}) - \int_0^x (a-1)t^{a-2}dt + \int_0^x (a-1)t^{a-2}e^{-t}dt$$

$$= x^{a-1}(1-e^{-x}) - (a-1)\frac{t^{a-1}}{a-1}\Big|_0^x + (a-1)\int_0^x t^{a-2}e^{-t}dt$$

$$= x^{a-1}(1-e^{-x}) - x^{a-1} + (a-1)\gamma(a-1,x)$$

Therefore

$$\gamma(a,x) = -x^{a-1}e^{-x} + (a-1)\gamma(a-1,x)$$

We also have the ordinary gamma function

$$\Gamma(a) = \gamma(a,\infty)$$

and its recursion

$$\Gamma(a) = (a-1)\Gamma(a-1)$$

Taking $j = 0$, we have

$$I = \int_{-\infty}^{\infty} |K_i(t)|\,dt = \int_{-\infty}^{\infty} K_i(t)dt = 1 = I_0$$

$$J = \int_{-\infty}^{\infty} K_i(t)^2dt = \int_{-\infty}^{\infty} \frac{1}{2\pi\sigma_i^2} e^{-(t/\sigma_i)^2}dt$$

$$= \int_{-\infty}^{\infty} \frac{1}{2\pi\sigma_i^2} e^{-t^2}\sigma_i dt = \frac{1}{2\pi\sigma_i}\int_{-\infty}^{\infty} e^{-t^2}dt$$

$$= \frac{1}{2\pi\sigma_i\sqrt{2}}\int_{-\infty}^{\infty} e^{-½t^2}dt = \frac{1}{2\pi\sigma_i\sqrt{2}}\sqrt{2\pi} \cdot \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-½t^2}dt$$

$$= \frac{1}{2\sqrt{\pi}\,\sigma_i}$$

but

$$\sigma_i = \frac{i^{1/2}h}{3^{1/2}}$$

Therefore

$$J = \frac{1}{2\sqrt{\pi}} \cdot \frac{3^{1/2}}{i^{1/2}h} = \frac{J_0}{i^{1/2}h}$$

where

$$J_0 = \tfrac{1}{2}\sqrt{3/\pi}$$

Taking j = 1, we have

$$I = \int_{-\infty}^{\infty} |K_i'(t)|\,dt = \int_{-\infty}^{\infty} \frac{|t|}{\sigma_i^2} K_i(t)dt = \int_{-\infty}^{\infty} \frac{|t|}{\sigma_i^2} \cdot \frac{1}{\sqrt{2\pi}\,\sigma_i} e^{-\frac{1}{2}(t/\sigma_i)^2}dt$$

$$= 2\int_0^{\infty} \frac{t}{\sigma_i^3\sqrt{2\pi}} e^{-\frac{1}{2}(t/\sigma_i)^2}dt = 2\int_0^{\infty} \frac{\sigma_i t}{\sigma_i^3\sqrt{2\pi}} e^{-\frac{1}{2}t^2}\sigma_i dt$$

$$= \frac{2}{\sigma_i\sqrt{2\pi}} e^{-\frac{1}{2}t^2}\Big|_{\infty}^{0} = \frac{1}{\sigma_i}\sqrt{2/\pi} = \frac{3^{1/2}}{i^{1/2}h} \cdot \sqrt{2/\pi} = \frac{I_1}{i^{1/2}h}$$

where

$$I_1 = \sqrt{6/\pi}$$

$$J = \int_{-\infty}^{\infty} K_i'(t)^2dt = \int_{-\infty}^{\infty} \frac{t^2}{\sigma_i^4} K_i(t)^2dt = \int_{-\infty}^{\infty} \frac{t^2}{\sigma_i^4} \cdot \frac{1}{2\pi\sigma_i^2} e^{-(t/\sigma_i)^2}dt$$

$$= \int_{-\infty}^{\infty} \frac{\sigma_i^2t^2}{\sigma_i^4} \cdot \frac{1}{2\pi\sigma_i^2} e^{-t^2}\sigma_i dt = \frac{1}{2\pi\sigma_i^3} \int_{-\infty}^{\infty} t^2e^{-t^2}dt$$

$$= \frac{1}{2\pi\sigma_i^3} \cdot \frac{1}{2\sqrt{2}} \cdot \sqrt{2\pi} \cdot \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} t^2e^{-\frac{1}{2}t^2}dt$$

$$= \frac{1}{4\sqrt{\pi}\,\sigma_i^3} = \frac{1}{4\sqrt{\pi}} \cdot \frac{3^{3/2}}{i^{3/2}h^3} = \frac{J_1}{i^{3/2}h^3}$$

where

$$J_1 = \frac{3}{4}\sqrt{3/\pi}$$

Finally, taking $j = 2$, we have

$$I = \int_{-\infty}^{\infty} |K_i''(t)|\,dt = \int_{-\infty}^{\infty} \frac{1}{\sigma_i^2} \left| \left(\frac{t}{\sigma_i}\right)^2 - 1\right| K_i(t)\,dt$$

$$= 2\int_0^{\infty} \frac{1}{\sigma_i^2} \left| \left(\frac{t}{\sigma_i}\right)^2 - 1\right| \cdot \frac{1}{\sqrt{2\pi}\,\sigma_i}\, e^{-\frac{1}{2}(t/\sigma_i)^2} dt = 2\int_0^{\infty} \frac{1}{\sigma_i^2} \left| t^2 - 1\right| \cdot \frac{1}{\sqrt{2\pi}\,\sigma_i}\, e^{-\frac{1}{2}t^2}\sigma_i\,dt$$

$$= \frac{1}{\sigma_i^2}\sqrt{2/\pi} \int_0^{\infty} |t^2-1|\, e^{-\frac{1}{2}t^2}dt = \frac{1}{\sigma_i^2}\sqrt{2/\pi}\left\{\int_0^1 (1-t^2)e^{-\frac{1}{2}t^2}dt + \int_1^{\infty} (t^2-1)e^{-\frac{1}{2}t^2}dt\right\}$$

Making the change of variable

$$u = \tfrac{1}{2}t^2$$

$$t = (2u)^{\frac{1}{2}}$$

$$dt = \tfrac{1}{2}(2u)^{-\frac{1}{2}}2du = (2u)^{-\frac{1}{2}}du$$

$$I = \frac{1}{\sigma_i^2}\sqrt{2/\pi}\left\{\int_0^{\frac{1}{2}} (1-2u)e^{-u}(2u)^{-\frac{1}{2}}du + \int_{\frac{1}{2}}^{\infty} (2u-1)e^{-u}(2u)^{-\frac{1}{2}}du\right\}$$

$$I = \frac{1}{\sigma_i^2}\sqrt{2/\pi}\left\{\int_0^{\frac{1}{2}} ((2u)^{-\frac{1}{2}} - (2u)^{\frac{1}{2}})e^{-u}du + \int_{\frac{1}{2}}^{\infty} ((2u)^{\frac{1}{2}} - (2u)^{-\frac{1}{2}})e^{-u}du\right\}$$

$$= \frac{1}{\sigma_i^2}\sqrt{2/\pi}\left\{2^{-\frac{1}{2}}\gamma(\tfrac{1}{2},\tfrac{1}{2}) - 2^{\frac{1}{2}}\gamma(\tfrac{3}{2},\tfrac{1}{2}) + 2^{\frac{1}{2}}(\Gamma(\tfrac{3}{2})-\gamma(\tfrac{3}{2},\tfrac{1}{2})) - 2^{-\frac{1}{2}}(\Gamma(\tfrac{1}{2}) - \gamma(\tfrac{1}{2},\tfrac{1}{2}))\right\}$$

$$= \frac{1}{\sigma_i^2}\sqrt{2/\pi}\left\{2^{\frac{1}{2}}\gamma(\tfrac{1}{2},\tfrac{1}{2}) - 2^{3/2}\gamma(\tfrac{3}{2},\tfrac{1}{2}) + 2^{\frac{1}{2}}\Gamma(\tfrac{3}{2}) - 2^{-\frac{1}{2}}\Gamma(\tfrac{1}{2})\right\}$$

$$= \frac{1}{\sigma_i^2}\sqrt{2/\pi}\left\{2^{\frac{1}{2}}\gamma(\tfrac{1}{2},\tfrac{1}{2}) - 2^{3/2}(-(\tfrac{1}{2})^{\frac{1}{2}}e^{-\frac{1}{2}}+\tfrac{1}{2}\gamma(\tfrac{1}{2},\tfrac{1}{2})) + 2^{\frac{1}{2}}\cdot\tfrac{1}{2}\Gamma(\tfrac{1}{2}) - 2^{-\frac{1}{2}}\Gamma(\tfrac{1}{2})\right\}$$

$$= \frac{1}{\sigma_i^2}\sqrt{2/\pi}\cdot 2e^{-\frac{1}{2}} = \frac{2}{\sigma_i^2}\sqrt{2/\pi e} = 2\cdot\frac{3}{ih^2}\sqrt{2/\pi e} = \frac{I_2}{ih^2}$$

where

$$I_2 = 6\sqrt{2/\pi e}$$

Now

$$J = \int_{-\infty}^{\infty} K_i''(t)^2 dt = \int_{-\infty}^{\infty} \frac{1}{\sigma_i^4}\left(\left(\frac{t}{\sigma_i}\right)^2 - 1\right)^2 K_i(t)^2 dt$$

$$= \int_{-\infty}^{\infty} \frac{1}{\sigma_i^4}\left(\left(\frac{t}{\sigma_i}\right)^2 - 1\right)^2 \cdot \frac{1}{2\pi\sigma_i^2} e^{-(t/\sigma_i)^2} dt$$

$$= \int_{-\infty}^{\infty} \frac{1}{\sigma_i^4} (t^2-1)^2 \cdot \frac{1}{2\pi\sigma_i^2} e^{-t^2}\sigma_i dt$$

$$= \frac{1}{\pi\sigma_i^5} \int_0^{\infty} (t^2-1)^2 e^{-t^2} dt$$

Making the change of variable

$$t^2 = u$$

$$t = u^{1/2}$$

$$dt = 1/2\, u^{-1/2} du$$

$$J = \frac{1}{\pi\sigma_i^5} \int_0^{\infty} (u-1)^2 e^{-u} \cdot 1/2\, u^{-1/2} du = \frac{1}{2\pi\sigma_i^5} \int_0^{\infty} u^{-1/2}(u^2-2u+1)e^{-u} du$$

$$= \frac{1}{2\pi\sigma_i^5} \int_0^{\infty} (u^{3/2} - 2u^{1/2} + u^{-1/2}) e^{-u} du$$

Therefore

$$J = \frac{1}{2\pi\sigma_i^5} (\Gamma(5/2) - 2\Gamma(3/2) + \Gamma(1/2)) = \frac{1}{2\pi\sigma_i^5} (3/2 \cdot 1/2\, \Gamma(1/2) - 2 \cdot 1/2\, \Gamma(1/2) + \Gamma(1/2))$$

but

$$\Gamma(1/2) = \sqrt{\pi}$$

Therefore

$$J = \frac{1}{2\pi\sigma_i^5} \cdot 3/4 \sqrt{\pi} = \frac{3}{8\sqrt{\pi}\ \sigma_i^5} = \frac{3}{8\sqrt{\pi}} \cdot \frac{3^{5/2}}{i^{5/2}h^5} = \frac{J_2}{i^{5/2}h^5}$$

where

$$J_2 = \frac{27}{8}\sqrt{3/\pi}$$

Summarizing these results for I and J, we have

$$I = \frac{I_j}{(h\sqrt{i})^j}$$

$$I_0 = 1 \quad , \quad I_1 = \sqrt{6/\pi} \quad , \quad I_2 = 6\sqrt{2/\pi e}$$

$$J = \frac{J_j}{(h\sqrt{i})^{2j+1}}$$

$$J_0 = \tfrac{1}{2}\sqrt{3/\pi} \quad , \quad J_1 = 3/4\sqrt{3/\pi} \quad , \quad J_2 = \frac{27}{8}\sqrt{3/\pi}$$

Our approximate global bound on q_j becomes

$$q_j^2 \lesssim \frac{1}{L}\int_0^L \left\{\frac{ih^2}{6}\left(\left|f^{(j+2)}(x)\right| + ih\left|f^{(j+3)}(x)\right|\right) + \frac{\tau^2 I_j}{8(h\sqrt{i})^j}\left(\left|f''(x)\right| + (ih+\tau)\left|f'''(x)\right|\right)\right\}^2 dx + \frac{\sigma^2\tau J_j}{(h\sqrt{i})^{2j+1}}$$

Note that all terms in the preceding bound either remain finite or $\to 0$ as $\tau \to 0$. Also note that for a given τ, some terms $\to \infty$ as $h \to 0$. What we would now like to do is to select an h (in terms of τ) which roughly minimizes this bound. We would then like all terms in the bound to $\to 0$ as τ (and h) $\to 0$.

Since we only need an h that roughly minimizes the bound, we can freely neglect small terms. We can begin by neglecting the $f^{(j+3)}$ and f''' terms as h, $\tau \to 0$. We then have

$$q_j^2 \lesssim \frac{1}{L}\int_0^L \left\{\frac{ih^2}{6}\left|f^{(j+2)}(x)\right| + \frac{\tau^2 I_j}{8(h\sqrt{i})^j}\left|f''(x)\right|\right\}^2 dx + \frac{\sigma^2\tau J_j}{(h\sqrt{i})^{2j+1}}$$

$$= \frac{i^2h^4}{36}\mu_{j+2,j+2} + \frac{ih^2\tau^2 I_j}{24(h\sqrt{i})^j}\mu_{2,j+2} + \frac{\tau^4 I_j^2}{64(h\sqrt{i})^{2j}}\mu_{2,2} + \frac{\sigma^2\tau J_j}{(h\sqrt{i})^{2j+1}}$$

where

$$\mu_{i,j} = \frac{1}{L}\int_0^L \left|f^{(i)}(x)\, f^{(j)}(x)\right| dx$$

Therefore

$$q_j^2 \lesssim \frac{1}{36} i^2 h^4 \mu_{j+2,j+2} + \frac{1}{24} i^{1-j/2} h^{2-j} \tau^2 I_j \mu_{2,j+2}$$

$$+ \frac{1}{64} \tau^4 h^{-2j} i^{-j} I_j^2 \mu_{2,2} + h^{-(2j+1)} i^{-(j+\frac{1}{2})} \sigma^2 \tau J_j$$

$$= a_1 h^4 + a_2 h^{2-j} \tau^2 + a_3 h^{-2j} \tau^4 + a_4 h^{-(2j+1)} \tau$$

where

$$a_1 = \frac{1}{36} i^2 \mu_{j+2,j+2}$$

$$a_2 = \frac{1}{24} i^{1-j/2} I_j \mu_{2,j+2}$$

$$a_3 = \frac{1}{64} i^{-j} I_j^2 \mu_{2,2}$$

$$a_4 = i^{-(j+\frac{1}{2})} \sigma^2 J_j$$

Differentiating this bound with respect to h and setting the result equal to zero gives

$$4a_1 h^3 + (2-j) a_2 h^{1-j} \tau^2 - 2j a_3 h^{-(2j+1)} \tau^4 - (2j+1) a_4 h^{-(2j+2)} \tau = 0$$

Multiplying through by h^{2j+2} gives

$$4a_1 h^{2j+5} + (2-j) a_2 h^{j+3} \tau^2 - 2j a_3 h \tau^4 - (2j+1) a_4 \tau = 0$$

Clearly, $h = 0$ if $\tau = 0$, but we would like an h in terms of small but finite τ. It seems that as far as τ is concerned, we should be able to neglect the a_2 and a_3 terms of the last equation. We will now do this and subsequently show that it is justified. Neglecting the second and third terms gives us

$$4a_1 h^{2j+5} - (2j+1) a_4 \tau = 0$$

Therefore

$$h = \left(\frac{(2j+1)a_4}{4a_1} \tau\right)^{\frac{1}{2j+5}} = c\tau^{\frac{1}{2j+5}}$$

where

$$c = \left(\frac{(2j+1)a_4}{4a_1}\right)^{\frac{1}{2j+5}} = \left(\frac{(2j+1)\, i^{-(j+\frac{1}{2})}\sigma^2 J_j}{1/9\ i^2 \mu_{j+2,j+2}}\right)^{\frac{1}{2j+5}}$$

$$= \left(\frac{9(2j+1)\sigma^2 J_j}{i^{j+5/2}\mu_{j+2,j+2}}\right)^{\frac{1}{2j+5}} = \frac{1}{\sqrt{i}}\left(\frac{9(2j+1)\sigma^2 J_j}{\mu_{j+2,j+2}}\right)^{\frac{1}{2j+5}}$$

Inserting the value for h back into the equation in which we neglected the second and third terms gives us

$$4a_1 c^{2j+5}\tau + (2-j)a_2\tau^2 c^{j+3}\tau^{\frac{j+3}{2j+5}} - 2ja_3\tau^4 c\tau^{\frac{1}{2j+5}} - (2j+1)a_4\tau = 0$$

or

$$4a_1 c^{2j+5}\tau + (2-j)a_2 c^{j+3}\tau^{\frac{5j+13}{2j+5}} - 2ja_3 c\tau^{\frac{8j+21}{2j+5}} - (2j+1)a_4\tau = 0$$

and we see that indeed, the a_2 and a_3 terms are asymptotically smaller (as $\tau \to 0$) than the two terms retained (the a_1 and a_4 terms). Also, for $j = 0$, the a_3 term is zero and for $j = 2$, the a_2 term is zero.

We now insert our (roughly) optimal value for h into our previous bound expression. The bound is

$$q_j^2 \lesssim a_1 h^4 + a_2 h^{2-j}\tau^2 + a_3 h^{-2j}\tau^4 + a_4 h^{-(2j+1)}\tau$$

$$= a_1 c^4 \tau^{\frac{4}{2j+5}} + a_2\tau^2 c^{2-j}\tau^{\frac{2-j}{2j+5}} + a_3\tau^4 c^{-2j}\tau^{\frac{-2j}{2j+5}} + a_4\tau c^{-(2j+1)}\tau^{\frac{-2j-1}{2j+5}}$$

$$= a_1 c^4 \tau^{\frac{4}{2j+5}} + a_2 c^{2-j}\tau^{\frac{3j+12}{2j+5}} + a_3 c^{-2j}\tau^{\frac{6j+20}{2j+5}} + a_4 c^{-(2j+1)}\tau^{\frac{4}{2j+5}}$$

It is interesting to simplify the coefficients of the powers of τ in this last bound and note that they are completely independent of i (the amount of smoothing).

Let

$$k = \left(\frac{9(2j+1)\sigma^2 J_j}{\mu_{j+2,j+2}}\right)^{\frac{1}{2j+5}}$$

therefore $c = ki^{-\frac{1}{2}}$.

Now

$$a_1c^4 = \frac{1}{36} i^2\mu_{j+2,j+2} \cdot k^4i^{-2} = \frac{1}{36} k^4\mu_{j+2,j+2}$$

$$a_2c^{2-j} = \frac{1}{24} i^{1-j/2}I_j\mu_{2,j+2}k^{2-j}i^{-\frac{1}{2}(2-j)} = \frac{1}{24} I_jk^{2-j}\mu_{2,j+2}$$

$$a_3c^{-2j} = \frac{1}{64} i^{-j}I_j^2\mu_{2,2} \cdot k^{-2j}i^{-\frac{1}{2}(-2j)} = \frac{1}{64} I_j^2k^{-2j}\mu_{2,2}$$

$$a_4c^{-(2j+1)} = i^{-(j+\frac{1}{2})}\sigma^2J_ji^{\frac{1}{2}(2j+1)}k^{-(2j+1)} = \sigma^2J_jk^{-(2j+1)}$$

Our roughly optimal asymptotic error bound is

$$q_j^2 \lesssim \frac{1}{36} k^4\mu_{j+2,j+2}\tau^{\frac{4}{2j+5}} + \frac{1}{24} I_jk^{2-j}\mu_{2,j+2}\tau^{\frac{3j+12}{2j+5}}$$
$$+ \frac{1}{64} I_j^2k^{-2j}\mu_{2,2}\tau^{\frac{6j+20}{2j+5}} + \sigma^2J_jk^{-(2j+1)}\tau^{\frac{4}{2j+5}}$$

Clearly, the second and third terms play a minor role as far as τ is concerned. We can therefore further simplify:

$$q_j^2 \lesssim (\frac{1}{36} k^4\mu_{j+2,j+2} + \sigma^2J_jk^{-(2j+1)})\tau^{\frac{4}{2j+5}}$$

Since

$$k = (\frac{9(2j+1)\sigma^2J_j}{\mu_{j+2,j+2}})^{\frac{1}{2j+5}}$$

we have

$$q_j^2 \lesssim \left(\frac{1}{36}\,\mu_{j+2,j+2}\left(\frac{9(2j+1)\sigma^2 J_j}{\mu_{j+2,j+2}}\right)^{\frac{4}{2j+5}} + \sigma^2 J_j\left(\frac{9(2j+1)\sigma^2 J_j}{\mu_{j+2,j+2}}\right)^{-\frac{2j+1}{2j+5}}\right)\tau^{\frac{4}{2j+5}}$$

$$= \frac{1}{36}\,\mu_{j+2,j+2}^{\frac{2j+1}{2j+5}}(9(2j+1)\sigma^2\tau J_j)^{\frac{4}{2j+5}} + (\sigma^2\tau J_j)^{\frac{4}{2j+5}}\mu_{j+2,j+2}^{\frac{2j+1}{2j+5}}(9(2j+1))^{-\frac{2j+1}{2j+5}}$$

$$= \mu_{j+2,j+2}^{\frac{2j+1}{2j+5}}(9(2j+1)\sigma^2\tau J_j)^{\frac{4}{2j+5}}\left(\frac{1}{36} + \frac{1}{9(2j+1)}\right)$$

Therefore

$$q_j^2 \lesssim \frac{1}{36}\left(\frac{2j+5}{2j+1}\right)\mu_{j+2,j+2}^{\frac{2j+1}{2j+5}}(9(2j+1)\sigma^2\tau J_j)^{\frac{4}{2j+5}}$$

Recalling the expression for our nearly optical h value

$$h_j = \frac{1}{\sqrt{i}}\left(\frac{9(2j+1)\sigma^2\tau J_j}{\mu_{j+2,j+2}}\right)^{\frac{1}{2j+5}}$$

and defining the constants

$$M_j = (9(2j+1)J_j)^{\frac{1}{2j+5}}$$

and

$$N_j = \frac{1}{6}\left(\frac{2j+5}{2j+1}\right)^{1/2}(9(2j+1)J_j)^{\frac{2}{2j+5}}$$

we summarize

$$h_j = \frac{M_j}{\sqrt{i}}\left(\frac{\sigma^2\tau}{\mu_{j+2,j+2}}\right)^{\frac{1}{2j+5}}$$

$$q_j \lesssim N_j\mu_{j+2,j+2}^{\frac{2j+1}{4j+10}}(\sigma^2\tau)^{\frac{2}{2j+5}}$$

where $M_0 = 1.345$, $M_1 = 1.53$, $M_2 = 1.74$, and $N_0 = 0.674$, $N_1 = 0.597$, and $N_2 = 0.679$. Note that $q_j \to 0$, $h_j \to 0$, and $h_j/\tau \to \infty$ as $\tau \to 0$.

We now apply these two formulas to the particular case of a sinusoidal function

$$f(t) = A \sin \omega t$$

First, we can easily compute that

$$\mu_{j+2,j+2} = \frac{A^2\omega^{2j+4}}{2}$$

We then have

$$q_j \lesssim N_j\left(\frac{A^2\omega^{2j+4}}{2}\right)^{\frac{2j+1}{4j+10}}(\sigma^2\tau)^{\frac{2}{2j+5}}$$

If we now define the error-to-noise ratio e to be q_j/σ and the signal-to-noise ratio s to be A/σ, we get

$$q_j \lesssim N_j\left(\frac{\sigma^2 s^2\omega^{2j+4}}{2}\right)^{\frac{2j+1}{4j+10}}(\sigma^2\tau)^{\frac{2}{2j+5}}$$

$$= N_j\sigma^{\frac{4j+2}{4j+10} + \frac{4}{2j+5}}\left(\frac{s^2\omega^{2j+4}}{2}\right)^{\frac{2j+1}{4j+10}}\tau^{\frac{2}{2j+5}}$$

Therefore

$$e \lesssim N_j\left(\frac{s^2\omega^{2j+4}}{2}\right)^{\frac{2j+1}{4j+10}}\tau^{\frac{2}{2j+5}}$$

To insure that e is bounded above by some specified number E, it is sufficient that

$$N_j\left(\frac{s^2\omega^{2j+4}}{2}\right)^{\frac{2j+1}{4j+10}}\tau^{\frac{2}{2j+5}} = E$$

or

$$\tau = \left(\frac{E}{N_j}\right)^{\frac{2j+5}{2}}\left(\frac{2}{s^2\omega^{2j+4}}\right)^{\frac{2j+1}{4}}$$

but

$$h_j = \frac{M_j}{\sqrt{i}}\left(\frac{\sigma^2\tau}{\mu_{j+2,j+2}}\right)^{\frac{1}{2j+5}} = \frac{M_j}{\sqrt{i}}\left(\frac{\sigma^2\tau}{\frac{A^2\omega^{2j+4}}{2}}\right)^{\frac{1}{2j+5}} = \frac{M_j}{\sqrt{i}}\left(\frac{2\tau}{s^2\omega^{2j+4}}\right)^{\frac{1}{2j+5}}$$

Inserting the previously computed value of τ into this expression for h_j gives

$$h_j = \frac{M_j}{\sqrt{i}} \left(\left(\frac{2}{s^2\omega^{2j+4}}\right)\left(\frac{E}{N_j}\right)^{\frac{2j+5}{2}} \left(\frac{2}{s^2\omega^{2j+4}}\right)^{\frac{2j+1}{4}} \right)^{\frac{1}{2j+5}}$$

$$= \frac{M_j}{\sqrt{i}} \left(\left(\frac{2}{s^2\omega^{2j+4}}\right)^{\frac{2j+5}{4}} \left(\frac{E}{N_j}\right)^{\frac{2j+5}{2}} \right)^{\frac{1}{2j+5}} = \frac{M_j}{\sqrt{i}} \left(\frac{2}{s^2\omega^{2j+4}}\right)^{\frac{1}{4}} \left(\frac{E}{N_j}\right)^{\frac{1}{2}}$$

Therefore

$$h_j = M_j\left(\frac{E}{isN_j}\right)^{\frac{1}{2}} \left(\frac{2}{\omega^{2j+4}}\right)^{\frac{1}{4}}$$

For a sinusoidal function, we may therefore estimate the needed sampling interval τ and window parameter h, given the desired error-to-noise ratio E, the signal-to-noise ratio s, the amount of smoothing i, the frequency ω, and the derivative index, j.

ERROR ANALYSIS WITHOUT NOISE

Recall from the last section that the approximate asymptotic error bound on the global error is given by

$$q_j^2 \lesssim a_1h^4 + a_2h^{2-j}\tau^2 + a_3h^{-2j}\tau^4 + a_4h^{-(2j+1)}\tau$$

and that setting the derivative of this bound with respect to h equal to zero yields (implicitly) the optimal window parameter

$$4a_1h^3 + (2-j)a_2h^{1-j}\tau^2 - 2ja_3h^{-(2j+1)}\tau^4 - (2j+1)a_4h^{-(2j+2)}\tau = 0$$

where

$$a_1 = \frac{1}{36} i^2\mu_{j+2,j+2}$$

$$a_2 = \frac{1}{24} i^{1-j/2}I_j\mu_{2,j+2}$$

$$a_3 = \frac{1}{64} i^{-j} I_j{}^2 \mu_{2,2}$$

$$a_4 = i^{-(j+\frac{1}{2})} \sigma^2 J_j$$

In the presence of noise, the a_1 and a_4 terms turned out to be the most significant, but without noise, the a_4 term is zero and we are left with

$$4a_1h^3 + (2-j)a_2h^{1-j}\tau^2 - 2ja_3h^{-(2j+1)}\tau^4 = 0$$

If $j = 0$, we have

$$4a_1h^3 + 2a_2h\tau^2 = 0$$

and we see that there is no real optimal h.

If $j = 1$, we have

$$4a_1h^3 + a_2\tau^2 - 2a_3h^{-3}\tau^4 = 0$$

or

$$4a_1h^6 + a_2\tau^2h^3 - 2a_3\tau^4 = 0$$

There are no dominant terms in this equation, so we may not neglect any. Solving this quadratic for h^3 gives

$$h^3 = \frac{\tau^2}{8a_1} \{-a_2 + (a_2{}^2+32a_1a_3)^{\frac{1}{2}}\}$$

If $j = 2$, we have

$$4a_1h^3 - 4a_3h^{-5}\tau^4 = 0$$

or

$$a_1h^8 = a_3\tau^4$$

Therefore

$$h = \left(\frac{a_3}{a_1}\right)^{1/8} \tau^{\frac{1}{2}}$$

Inserting the expressions for the a's gives

$$h = \left(\frac{9I_2{}^2\mu_{2,2}}{16\mu_{4,4}}\right)^{1/8} \left(\frac{\tau}{i}\right)^{\frac{1}{2}}$$

and

$$q_2^2 \lesssim \frac{I_2}{24}(\mu_{2,4}+(\mu_{2,2}\mu_{4,4})^{1/2})\tau^2$$

We see that even without noise, there are optimal window parameters and corresponding error bounds for derivatives.

BEST ANALYTIC ERROR BOUND

In this section, we show that the previously obtained upper bound on the analytic error in the jth derivative of the ith smooth of a smooth function is the best possible, i.e., the smallest. We will streamline the error analysis by making use of the kernel functions and their properties

$$D^jS^if(x) = S^iD^jf(x) = S^if^{(j)}(x) = \int_{x-ih}^{x+ih} K_i(t-x)f^{(j)}(t)dt$$

$$= \int_{-ih}^{ih} K_i(t)f^{(j)}(t+x)dt = \int_{-ih}^{0} K_i(t)f^{(j)}(t+x)dt - \int_{ih}^{0} K_i(t)f^{(j)}(t+x)dt$$

Using integration-by-parts, we have

$$D^jS^if(x) = f^{(j)}(x)\int_{-ih}^{0} K_i(t)dt - \int_{-ih}^{0} f^{(j+1)}(t+x)\int_{-ih}^{t} K_i(u)dudt$$

$$- \{f^{(j)}(x)\int_{ih}^{0} K_i(t)dt - \int_{ih}^{0} f^{(j+1)}(t+x)\int_{ih}^{t} K_i(u)dudt\}$$

Let

$$I(t) = \int_{-ih}^{t} K_i(u)du$$

Therefore

$$D^jS^if(x) = f^{(j)}(x)\int_{-ih}^{ih} K_i(t)dt - \int_{-ih}^{0} f^{(j+1)}(t+x)I(t)dt$$

$$+ \int_{ih}^{0} f^{(j+1)}(t+x)(I(t)-I(ih))dt$$

Then

$$D^j S^i f(x) - f^{(j)}(x) = -\int_{-ih}^{0} f^{(j+1)}(t+x) I(t)dt + \int_{ih}^{0} f^{(j+1)}(t+x)(I(t)-1)dt$$

Again, integrating-by-parts,

$$D^j S^i f(x) - f^{(j)}(x) = -\{f^{(j+1)}(x) \int_{-ih}^{0} I(t)dt - \int_{-ih}^{0} f^{(j+2)}(t+x) \int_{-ih}^{t} I(u)dudt\}$$

$$+ f^{(j+1)}(x) \int_{ih}^{0} (I(t)-1)dt - \int_{ih}^{0} f^{(j+2)}(t+x) \int_{ih}^{t} (I(u)-1)dudt$$

$$= f^{(j+1)}(x)\{-\int_{-ih}^{0} I(t)dt + \int_{0}^{ih} (1-I(t))dt\} + \int_{-ih}^{0} f^{(j+2)}(t+x) \int_{-ih}^{t} I(u)dudt$$

$$+ \int_{0}^{ih} f^{(j+2)}(t+x) \int_{t}^{ih} (1-I(u))dudt$$

Now

$$I(t) = \int_{-ih}^{t} K_i(u)du$$

therefore

$$I(-t) = \int_{-ih}^{-t} K_i(u)du = -\int_{ih}^{t} K_i(-u)du$$

$$= \int_{t}^{ih} K_i(u)du = I(ih) - I(t) = 1 - I(t)$$

Therefore

$$D^j S^i f(x) - f^{(j)}(x) = f^{(j+1)}(x)\{-\int_{-ih}^{0} I(t)dt + \int_{0}^{ih} I(-t)dt\}$$

$$+ \int_{-ih}^{0} f^{(j+2)}(t+x) \int_{-ih}^{t} I(u)dudt + \int_{0}^{ih} f^{(j+2)}(t+x) \int_{t}^{ih} I(-u)dudt$$

$$= f^{(j+1)}(x)\{-\int_{-ih}^{0} I(t)dt + \int_{-ih}^{0} I(t)dt\} + \int_{-ih}^{0} f^{(j+2)}(t+x) \int_{-ih}^{t} I(u)dudt$$

$$+ \int_{0}^{ih} f^{(j+2)}(t+x) \int_{-ih}^{-t} I(u)dudt$$

but

$$\int_0^{ih} f^{(j+2)}(t+x)\int_{-ih}^{-t} I(u)\,du\,dt = -\int_0^{-ih} f^{(j+2)}(-t+x)\int_{-ih}^{t} I(u)\,du\,dt$$

$$= \int_{-ih}^{0} f^{(j+2)}(x-t)\int_{-ih}^{t} I(u)\,du\,dt$$

We thus have

$$D^jS^if(x) - f^{(j)}(x) = \int_{-ih}^{0} f^{(j+2)}(t+x)\int_{-ih}^{t} I(u)\,du\,dt$$

$$+ \int_{-ih}^{0} f^{(j+2)}(x-t)\int_{-ih}^{t} I(u)\,du\,dt$$

Taking absolute values and using the usual norm, we get

$$|D^jS^if(x) - f^{(j)}(x)| \leq 2\|f^{(j+2)}\|_{(x;ih)}\int_{-ih}^{0}\int_{-ih}^{t} I(u)\,du\,dt$$

$$= 2\|f^{(j+2)}\|_{(x;ih)}\int_{-ih}^{0}\int_{-ih}^{t}\int_{-ih}^{u} K_i(s)\,ds\,du\,dt$$

By reversing the order of integration in the triple integral a couple of times, we get

$$\int_{-ih}^{0}\int_{-ih}^{t}\int_{-ih}^{u} K_i(s)\,ds\,du\,dt = \int_{-ih}^{0} \frac{s^2}{2} K_i(s)\,ds$$

$$= \frac{1}{4}\int_{-ih}^{ih} s^2K_i(s)\,ds = \frac{\sigma_i^2}{4} = \frac{ih^2}{12}$$

We finally get

$$|D^jS^if(x) - f^{(j)}(x)| \leq 2\|f^{(j+2)}\|_{(x;ih)} \cdot \frac{ih^2}{12} = \frac{ih^2}{6}\|f^{(j+2)}\|_{(x;ih)}$$

and we see that no better bound is possible.

A COMPUTATIONAL CONSIDERATION

To repeat, the ith smooth of function f is given by

$$S^i f(x) = \frac{1}{(2h)^i} \sum_{k=0}^{i} (-1)^k \binom{i}{k} f_i(x+(i-2k)h)$$

where

$$f_i(u) = \int_a^u f(t) \frac{(u-t)^{i-1}}{(i-1)!} dt$$

Now, for a given value of x, a is arbitrary, but if u is considerably different from a, the integral $f_i(u)$ can be quite large. This can lead to a major loss of significance through round-off error in the smoothing sum. To avoid this, we prevent $f_i(u)$ from becoming too large by selecting a equal to x.

Hence, we compute

$$f_i(u) = \int_x^u \phi_i(t)dt$$

where

$$\phi_i(t) = f(t) \frac{(u-t)^{i-1}}{(i-1)!}$$

Now, assume f(t) to be defined piecewise on some x mesh. Let $x_\ell \leq x \leq x_{\ell+1}$ and $x_m \leq u \leq x_{m+1}$ where $\ell \leq m$,

$$(\text{if } \ell > m,\ f_i(u) = -\int_u^x \phi_i(t)dt)$$

$$\text{if } m = \ell,\ f_i(u) = \int_x^u \phi_i(t)dt$$

$$\text{if } m = \ell+1,\ f_i(u) = \int_x^{x_{\ell+1}} \phi_i(t)dt + \int_{x_{\ell+1}}^u \phi_i(t)dt$$

if $m \geq \ell+2$,

$$f_i(u) = \int_x^{x_{\ell+1}} \phi_i(t)dt + \int_{x_{\ell+1}}^{x_{\ell+2}} \phi_i(t)dt$$

$$+ \dots + \int_{x_{m-1}}^{x_m} \phi_i(t)dt + \int_{x_m}^{u} \phi_i(t)dt$$

$$= \int_x^{x_{\ell+1}} \phi_i(t)dt + \sum_{n=\ell+1}^{m-1} \int_{x_n}^{x_{n+1}} \phi_i(t)dt + \int_{x_m}^{u} \phi_i(t)dt$$

We therefore need to compute integrals of the form

$$\int_\alpha^\beta \phi_i(t)dt \text{ where } x_p \leq \alpha,\beta \leq x_{p+1}$$

In the special case when f(t) is piecewise linear and continuous, we have

$$f(t) = y_p + \frac{t - x_p}{x_{p+1} - x_p} (y_{p+1} - y_p) \text{ for } x_p \leq t \leq x_{p+1}$$

or

$$f(t) = y_p + q_p(t-x_p)$$

where

$$q_p = \frac{y_{p+1} - y_p}{x_{p+1} - x_p}$$

Therefore

$$\phi_i(t) = (y_p + q_p(t-x_p)) \frac{(u-t)^{i-1}}{(i-1)!}$$

and

$$\int_\alpha^\beta \phi_i(t)dt = \int_\alpha^\beta (y_p + q_p(t-u+u-x_p)) \frac{(u-t)^{i-1}}{(i-1)!} dt$$

$$\int_\alpha^\beta \phi_i(t)dt = \frac{(y_p + q_p(u-x_p))}{(i-1)!} \int_\alpha^\beta (u-t)^{i-1}dt$$

$$- \frac{q_p}{(i-1)!} \int_\alpha^\beta (u-t)^i dt$$

$$= \frac{(y_p + q_p(u-x_p))}{i!} ((u-\alpha)^i - (u-\beta)^i)$$

$$+ \frac{iq_p}{(i+1)!} ((u-\beta)^{i+1} - (u-\alpha)^{i+1})$$

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